Weakly interacting two-dimensional system of dipoles: limitations of mean-field theory

G.E. Astrakharchik, J. Boronat, and J. Casulleras
Departament de Física i Enginyeria Nuclear, Campus Nord B4-B5, Universitat Politècnica de Catalunya, E-08034 Barcelona, Spain

I.L. Kurbakov and Yu.E. Lozovik
Institute of Spectroscopy, 142190 Troitsk, Moscow region, Russia
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We consider a homogeneous 2D Bose gas with repulsive dipole-dipole interactions. The ground-state equation of state, calculated using the Diffusion Monte Carlo method, shows quantitative differences with predictions of commonly used Gross-Pitaevskii mean-field theory. The static structure factor, pair distribution function and condensate fraction are calculated in a wide range of the gas parameter. Differences with mean-field theory are reflected in the frequency of the lowest "breathing" mode for harmonically trapped systems.

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The study of quasi-two-dimensional Bose gases at ultra-low temperatures has become a very active area of research. The role of correlations and quantum fluctuations is greatly enhanced in reduced dimensionality making a two-dimensional (2D) system well suited for studying beyond mean-field effects. The superfluid-normal phase transition occurs at a finite-temperature and follows the peculiar scenario of Berezinskii, Kosterlitz, Thouless [1]. On the contrary, the system undergoes Bose-Einstein condensation (BEC) only at zero temperature[2], since long-wavelength phase fluctuations destroy long-range order. The analytical descriptions of 2D systems include mean-field Gross-Pitaevskii (GPE) theory [3, 4], beyond mean-field approaches [5, 6], and numerical methods [7, 8, 9].

Recently, Bose-Einstein condensation was achieved in ^{52}Cr atoms [10]. Chromium possesses a large permanent magnetic moment making the experimental observation of effects of dipole-dipole interactions possible [11]. Moreover, by tuning its s-wave scattering length by a Feshbach resonance, one can realize a system with purely dipolar interactions. The first study of the Feshbach resonances in ^{52}Cr atoms appeared recently [12]. As shown in Ref. [13], this procedure would permit to tune the effective quasi-two-dimensional coupling constant g_{2D}. In addition, the Bose-Einstein condensation of 2D dipolar excitons in quantum wells was recently observed in luminescence experiments [14]. In two coupled quantum wells, one containing only holes, and the other only electrons, holes and electrons might couple forming indirect excitons. Alternatively, the exciton dipole moment can be induced by normal electric field in a single quantum well. Spatial separation between hole and electron suppresses recombination and greatly increases the lifetime of an exciton. If the separation between excitons are greater than the electron - hole separation D, an indirect exciton can be approximated as a boson with dipolar moment oriented perpendicularly to the plane.

A homogeneous system of N dipoles is described by the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2M}\sum_{i=1}^{N}\Delta_i + \frac{C_{dd}}{4\pi}\sum_{j<k}\frac{1}{|\mathbf{r_j}-\mathbf{r_k}|^3}, \qquad (1)$$

where M is the mass of a dipole. The coupling constant C_{dd} depends on the nature of the dipolar interaction. For cold atoms with large permanent magnetic moment m one has $C_{dd} = \mu_0 m^2$, where μ_0 is the permeability of free space. If the dipole moment is induced by an electric field E, the coupling constant is $C_{dd} = E^2\alpha^2/\epsilon_0$, where α is the static polarizability and ϵ_0 the permittivity of free space. In the case of excitons $C_{dd} = e^2D^2/\varepsilon$, where e is the electron charge and ε is the dielectric constant of the semiconductor.

We suppose that the atoms are confined in a very tight pancake trap, so that dynamically the system is two-dimensional, and the dipole moments are aligned perpendicularly to the plane. This stabilizes the system since interactions are purely repulsive.

The properties of Hamiltonian (1) are governed by the two-dimensional gas parameter na^2, n being the 2D density and a the 2D s-wave scattering length. The limit $na^2 \to 0$ corresponds to a weakly interacting regime where the mean-field (MF) theory can be applied. The MF energy per particle is proportional to the coupling constant: $E^{MF}/N = gn/2$. The leading contribution to the purely 2D coupling constant was first obtained by Shick[3] and rigorously derived for GPE by Lieb *et al.*[4]

$$g_{2D}^{MF} = \frac{4\pi\hbar^2}{M}\frac{1}{|\ln na^2|} \qquad (2)$$

A peculiarity of a two-dimensional system is that the coupling constant depends on density, while it is independent of density in three- and one- dimensional systems. This factor causes particular energetic properties (for example, in the frequencies of collective oscillations). Calculation of subleading corrections to MF (2) is a difficult and

long-standing problem and it was addressed by different authors [5] giving sometimes controversial results.

In a 2D system a Bose-Einstein condensate can only be formed at zero temperature. The system is completely condensed in the limit $na^2 \to 0$, while in a denser system the condensate density n_0 gets depleted. The departure from the fully condensed state is given by the perturbative expression [3]

$$\frac{n_0}{n} = 1 - \frac{1}{|\ln na^2|} + \mathcal{O}\left(\frac{1}{\ln^2 na^2}\right) \tag{3}$$

For small momenta the excitation spectrum is linear $\mathcal{E}_k = \hbar|k|c$, with c being the speed of sound, which corresponds to having phonons in the system. This defines a linear behavior of the static structure factor

$$S_k^{ph.} = \frac{\hbar|k|}{2Mc}, \qquad |k|/n^{1/2} \ll 1 \tag{4}$$

in agreement with Feynman formula [15] that relates the excitation spectrum to the static structure factor $\mathcal{E}_k = \hbar^2k^2/(2MS_k)$. Excitations at very high momenta $|k|/n^{1/2} \gg 1$ are free particles $\mathcal{E}_k = \hbar^2k^2/2M$ and $S_k = 1$. The intermediate behavior of the static structure factor at $|k|n^{1/2} \approx 1$ can be approximated in the weakly-interacting regime by assuming the Bogoliubov excitation spectrum $\mathcal{E}_k = \sqrt{\hbar^2k^2\mu/M + (\hbar^2k^2/2M)^2}$,

$$S_k^{Bog.} = \frac{|k|}{\sqrt{16\pi n/|\ln na^2| + k^2}}, \qquad na^2 \ll 1 \tag{5}$$

We analyze the ground-state properties of the system described by the Hamiltonian (1) resorting to the Diffusion Monte Carlo (DMC) technique. The guiding wave function is of Jastrow type, with a two-body correlation terms corresponding at short distances to a solution of the two-body scattering problem and smoothly matched to a long-range hydrodynamic asymptotics at larger distances (further details in Ref. [7]). The parameters of the guiding wave function are optimized by energy minimization in variational Monte Carlo calculations. The optimal guiding wave function is then used as an input to the DMC algorithm, which produces exact (apart from some statistical uncertainty) ground-state energies in a system of bosons. The pair distribution function and static structure factor are calculated using the technique of pure estimators [16]. The one-body density matrix is estimated using the extrapolated estimator using DMC and VMC results [16]. As finite-size effects are very important for the case of a dipolar interaction potential [7], we perform calculations with system sizes $N = 19; 25; 35; 50; 70; 100; 200$ and do extrapolation of the energy to the thermodynamic limit $N \to \infty$.

DMC results for the ground-state energy as a function of the gas parameter na^2 are reported in Fig. 1. In the inset, we make a direct comparison to the mean-field energy, Eq. (2). We note that while the MF description is

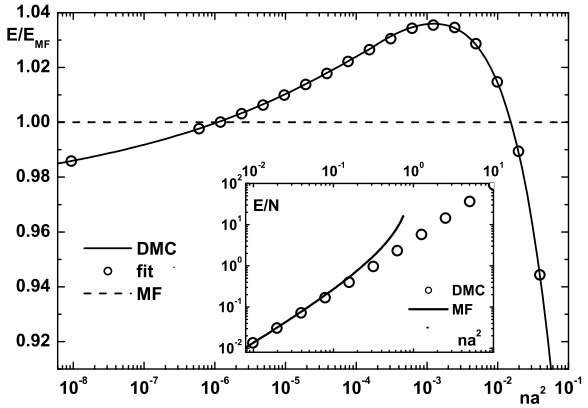

FIG. 1: Ground state energy per particle as a function of the gas parameter na^2. Inset: in units of $\hbar^2/(Ma^2)$, symbols - DMC data, line - mean-field energy E_{MF}, Eq. (2). Main figure: in units of E_{MF}, symbols - DMC data, solid line - best fit, Eq. (6), dashed line - mean-field energy.

in a qualitative agreement with our data up to large values of the gas parameter $na^2 \lesssim 0.1$, quantitatively there are noticeable differences. In order to test the quality of analytical equations of state we plot in Fig. 1 the energy in units of the MF energy. Even at the smallest considered density $na^2 = 10^{-8}$ MF theory does not provide a quantitatively correct result. The behavior at such low densities is expected to be universal and defined by the gas parameter. Indeed, the energy of dipoles is almost indistinguishable from the energy of both soft and hard spheres[17] when $na^2 < 10^{-6}$. It is worth noticing that the situation is different from the 3D case where there is a perfect agreement with MF for values of the gas parameter $n_{3D}a_{3D}^3 \lesssim 10^{-6}$ [18]. In a 1D system, the MF result is recovered with an accuracy better than 10^{-3} already for $n_{1D}|a_{1D}| \lesssim 10^{-3}$ [19]. The reason for such a difference is that in three- and one- dimensional systems the expansion comes in terms of the gas parameter, whereas in 2D the expansion is done in terms of $1/\ln na^2$, and corrections to the energy include slowly converging terms $\ln|\ln na^2|$. This means that for experimentally interesting densities $na^2 \gg 10^{-8}$, one must consider additional terms in the equation of state (2). We tested a number of equations of state present in the literature [5] and none of them is able to reproduce correctly the DMC value of the energy even at $na^2 = 10^{-8}$. Thus, the only remaining way to obtain a quantitatively correct description of a 2D dipolar gas is to perform a microscopic study. We fit the DMC equation of state in the density range $10^{-6} < na^2 < 10^3$ using the following function

$$\frac{E}{N} = \begin{cases} \frac{\hbar^2}{Ma^2}\exp(a_0 + a_1 l + a_2 l^2 + a_3 l^3 + a_4 l^4), & n > n_c \\ \frac{2\pi\hbar^2 n}{M}\left(b_0 + b_1 l + b_2 \ln l + b_3 \ln\ln l\right), & n \le n_c \end{cases} \tag{6}$$

where $l = |\ln na^2|$. The best fit gives $a_0 = 1.4552(4)$, $a_1 = -1.3033(1)$, $a_2 = 0.01267(2)$, $a_3 = 7.7(2)\cdot 10^{-5}$,

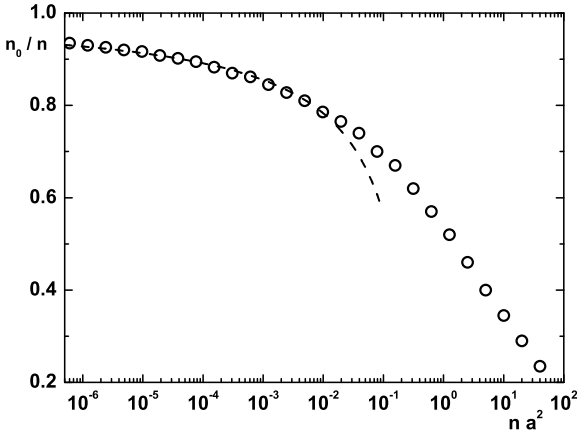

FIG. 2: Condensate fraction as a function of the gas parameter na^2, symbols - DMC data, dashed line - perturbative low density prediction, Eq. (3).

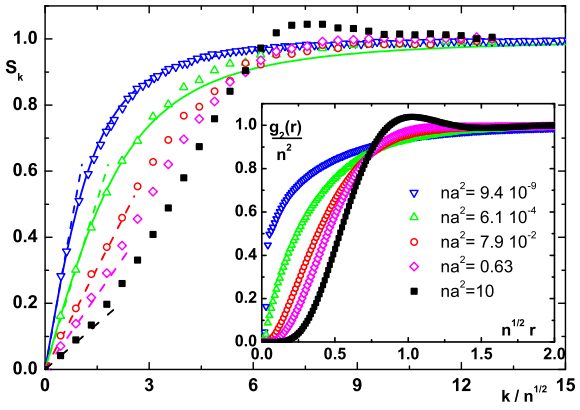

FIG. 3: Static structure factor: symbols - DMC data, dashed lines - the low-momenta phononic behavior, Eq. (4), solid lines - Feynman prediction assuming Bogoliubov excitation spectrum Eq. (5). Inset: pair distribution function. In descending order of the slope at $r = 0$: $na^2 = 9.4 \cdot 10^{-9}$; $6.1 \cdot 10^{-4}$; $7.9 \cdot 10^{-2}$; 0.63; 10

$a_4 = -2.18(4) \cdot 10^{-5}$, $b_0 = -2.225(20)$, $b_1 = 1$, $b_2 = 3.294(5)$, $b_3 = -6.65(1)$, $n_c = 1.8 \cdot 10^{-4}$. Numbers in parentheses indicate the uncertainty of the fitting procedure. The resulting curve is shown in Fig. 1.

The condensate fraction n_0/n is obtained from the non-diagonal long-range asymptotics of the one-body density matrix [7]. In Fig. 2, we plot results of n_0/n as a function of the gas parameter. We find that the predictions of Bogoliubov theory, Eq. (3), are in a good agreement in the weakly interacting regime. This should be contrasted with the energy, where the difference at the same density is significative. Nevertheless, at larger densities deviations are found. We note that at the densities of physical interest for excitonic systems $na^2 \approx 1 - 10$, the condensate is highly suppressed, making the applicability of the Gross-Pitaevskii equation, where the system is thought to be fully condensed, hardly possible. Moreover, in this regime it is expected that the universal description in terms of the s-wave scattering length breaks down and the properties of the system depend crucially on details of the potential.

In Fig. 3, we plot the static structure factor S_k calculated in a system with $N = 200$ particles in a wide range of the gas parameter $9.4 \cdot 10^{-9} \leq na^2 \leq 10$. The static structure factor is obtained as a Fourier transformation of the pair distribution function. The low-momentum part of S_k is in agreement with the linear phonon prediction (4), shown in Fig. 3 with short-dashed lines. The slope is proportional to the speed of sound c, which, in Fig. 3, is calculated from the fit (6). We see that for the two smallest considered densities Bogoliubov theory of weakly interacting Bose gas provides a relatively good description of the static structure factor. In the inset of Fig. 3 we show the characteristic behavior of the pair distribution function $g_2(r)$. In the regime of low densities $g_2(r)$ goes smoothly from zero (the dipole potential is highly repulsive when $r \to 0$) to the constant value $g_2(r) \to n^2, n^{1/2}|r| \gg 1$, which is a typical behavior for a liquid (gas). We note that in this regime at small distances the pair distribution function is proportional to the square of the two-body scattering solution $f_{TB}(r)$: $g_2(r) = const \cdot |f_{TB}(r)|^2$, while the coefficient of proportionality is a many-body property and can not be extracted from the two-body problem. At large densities $na^2 \approx 1$ a peak at mean interparticle distance $r = n^{-1/2}$ starts to be formed, which shows that the system is more correlated in this regime. Indeed, it was found[7, 8] that the system of dipoles experience a quantum phase transition to a crystal if the density is greatly increased.

Differences in the equation of state have consequences also in trapped systems, leading to different values of the release energy, the size of the cloud, *etc.* One of the most precise techniques, which can be used for testing the equation of state, is the measurement of the frequency of the "breathing" mode produced by a sudden change of the frequency of the harmonic trapping in the 2D plane. In order to calculate the frequency of this mode in a trapped system we have used the local density approximation (LDA) [20]. Within this approximation all properties depend on a characteristic parameter Na^2/a_{ho}^2, where a_{ho} is the oscillator length of the confinement in the 2D plane. The frequencies of the "breathing" mode in a 2D system were calculated in Ref. [20] using scaling approach and assuming that the amplitude of oscillations is small. In a symmetric trap this frequency is given by

$$\Omega^2 = -2\langle r^2 \rangle \Big/ \frac{\partial \langle r^2 \rangle}{\partial \omega^2} \qquad (7)$$

The mean square size of the cloud is calculated within

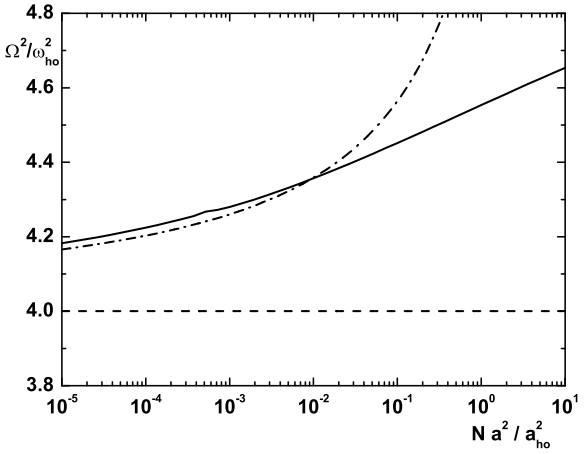

FIG. 4: Reduced square Ω^2/ω_{ho}^2 of the lowest monopole frequency ("breathing" mode) in an isotropic trap, calculated as Eq. (7), for the DMC (solid line), MF (dash-dotted line) equations of states as a function of LDA parameter. For comparison we plot $n \to 0$ asymptotic $\Omega = 2\omega_{ho}$ (dashed line).

LDA assuming that $\langle r^2 \rangle \gg a_{ho}^2$. This condition is easily satisfied if the number of dipoles in the trap N is large.

In Fig. 4, we show frequencies of the "breathing" mode Ω obtained for different equations of state. In the regime of weak interactions $Na^2/a_{ho}^2 \to 0$ the frequency goes asymptotically to a constant value $\Omega = 2\omega_{ho}$. This value corresponds to the mean-field result $\mu = gn$, with a coupling constant g independent of density[22]. Differently to three- and one- dimensional systems, the purely-two-dimensional regime of constant Ω can not be probably reached in experiments, since the system should be extremely dilute. Indeed, even for the smallest considered values of the LDA parameter $Na^2/a_{ho}^2 = 10^{-5}$ the square of the frequency $\Omega^2 \approx 4.2\omega_{ho}^2$ is considerably different from the limiting one. Already for this value of the LDA parameter we find differences between the DMC and mean-field equations of state. This discrepancy becomes more evident when the system enters into a regime of stronger interactions $Na^2/a_{ho}^2 \approx 10^{-1}$. On the other hand, in the characteristic densities of excitonic experiments $na^2 \approx 1 - 10$ the mean-field description, Eq. (2), fails completely and data should rely on DMC results. We note that differences of several percent can be resolved in present high-precision experiments with cold gases (see, for example, Ref. [21]).

In conclusion, we have performed a fully microscopic description of a weakly interacting system of dipoles using the DMC method. The ground-state equation of state, as well as results for the static structure factor, pair distribution function and condensate fraction are reported. It has been shown that Bogoliubov theory provides a good description of correlation functions in the dilute regime. For a harmonically trapped systems we calculate the frequency of the "breathing" mode using local density approximation. This frequency provides a sensitive tool for testing the equation of state and can be measured in near future in experiments. An important conclusion of the present work is the failure of the commonly used Gross-Pitaevskii mean-field theory (differently from 3D and 1D systems) to describe quantitatively energetic properties of a weakly interacting 2D system of dipoles. This failure is present already in the universal regime, *i.e.*, where the shape of the interaction potential is no longer important, suggesting that special care should be taken in the description of properties of any 2D dilute Bose system.

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